SEARCH REQUEST FORM

17/2014

Requestor's Serial Number: _______ Number: _______ / 0 / 0 C

NDV HE

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevent citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevent claim(s).

Point of Contact: Beverly Shears Technical Info. Specialist CM1 1E05 Tel: 308-4994

 $N^{2} = (H_{2} - (D_{1}^{2})^{2}) \times (H_{2} - (H_{3}^{2})^{2}) \times (H_{2} - (H_{3}^{2})^{2}) \times (H_{2} - (H_{3}^{2})^{2}) \times (H_{3} - (H_{3}^{2})$

to not broaden search

(135

STAFF USE ONLY

 Date completed:
 10-04-02
 Search Site

 Searcher:
 20-17 = 4954
 STIC

 Terminal time:
 12 CM-1

 Elapsed time:
 Pre-S
 Type f Search

 CPU time:
 N.A. Sequence

 Number of Searches:
 A.A. Sequence

 Number of Databases:
 Structure

 Search Site
 Vendors

 _____ STIC
 _____ IG

 _____ CM-1
 _____ STN

 _____ Pre-S
 _____ Dialog

 Type f Search
 _____ APS

 _____ N.A. Sequence
 ______ Geninfo

 A.A. Sequence
 SDC

Structure DARC/Questel
Bibliographic Other

VETLE 'REGISTRY' ENTERED AT 15:38:11 ON 04 OCT 2002)
STR

24 G2 0 CH2 Cb NO2 $CH2 \sim C = CH2$ 018 19 20 @21 22 23 SH 11 17 0 10 0 ∨ 0~ G1 13 14 15

VAR G1=18/21
VAR G2=H/CH3
REP G3=(1-6) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 8
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L9 1-SEA FILE=REGISTRY SSS FUL L7

100.0% PROCESSED 165 ITERATIONS

SEARCH TIME: 00.00.03

FILE 'HCAPLUS' ENTERED AT 15:45:34 ON 04 OCT 2002

L10 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

2002:449689 HCAPLUS

DOCUMENT NUMBER:

137:33162

TITLE:

L7

Process for the preparation of p-nitrobenzyl or

1 ANSWERS

allyl esters of 3-cyclic-ether substituted cephalosporins from trimethylphosphinic

compounds via an intramolecular Wittig reaction Colberg, Juan Carlos; Tucker, John Lloyd;

INVENTOR(S): Colberg, Juan Carlos; Tucker, John

Zenoni, Maurizio; Fogliato, Giovanni; Donadelli,

Alessandro

PATENT ASSIGNEE(S):

Pfizer Products Inc., USA PCT Int. Appl., 47 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

SOURCE:

1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

Searcher : Shears

ears 308-4994

```
KIND
                            DATE
                                           APPLICATION NO.
                                                             DATE
     PATENT NO.
                      ----
                            -----
                                           WO 2001-IB2181
                            20020613
                                                             20011119
     WO 2002046199
                       A1
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ,
             NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
             TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE,
             CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT,
             SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
                            20020618
                                           AU 2002-23929
                                                             20011119
     AU 2002023929
                       Α5
     US 2002099205
                            20020725
                                           US 2001-6579
                                                             20011204
                       A1
                                         US 2000-251018P
                                                          Ρ
                                                             20001204
PRIORITY APPLN. INFO.:
                                        WO 2001-IB2181
                                                          W
                                                             20011119
                         CASREACT 137:33162; MARPAT 137:33162
OTHER SOURCE(S):
```

GΙ

AB A process for the prepn. of I (R1 = p-nitrobenzyl, allyl; X = halo) via an intramol. Wittig reaction of II (R1 = p-nitrobenzyl, allyl; R2 = C1-6-alkyl, C6-10-aryl, C6-10-aryl-C1-6-alkyl, dithianyl) to prep. 3-cyclic-ether substituted derivs. of cephalosporins is described. Thus, III was treated with p-nitrobenzyl glyoxylate monohydrate followed by redn. of the intermediate with NaBH4. resulting hydroxy compd. was treated with p-toluenesulfonic acid followed by addn. of (S)-1-(tetrahydro-2-furanyl)ethanone, addn. of thionyl chloride, and finally trimethylphosphine to give the desired intermediate II (R1 = p-nitrobenzyl, R2 = PhCH2). Cyclization of II via an intramol. Wittig reaction was accomplished by refluxing for 16 h in THF. Addn. of phosphorus pentachloride and .alpha.-picoline in dichloromethane gave the free amine of I (R1 = p-nitrobenzyl). IT 436800-39-4P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic

preparation); PREP (Preparation); RACT (Reactant or reagent) (process for the prepn. of p-nitrobenzyl or allyl esters of 3-cyclic-ether substituted cephalosporins from

trimethylphosphinic compds. via an intramol. Wittig reaction)

436800-39-4 HCAPLUS RN

1-Azetidineacetic acid, .alpha.-hydroxy-2-mercapto-4-oxo-3-CN [(phenylacetyl)amino]-, (4-nitrophenyl)methyl ester, (2R, 3R)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN

THE RE FORMAT

'CAOLD' ENTERED AT 15:46:12 ON 04 OCT 2002 L11 0 S L9

FILE 'USPATFULL' ENTERED AT 15:46:18 ON 04 OCT 2002 L12 1 S L9

L12 ANSWER 1 OF 1 USPATFULL

ACCESSION NUMBER: 2002:186282 USPATFULL

Process and ester derivatives useful for TITLE:

preparation of cephalosporins

Colberg, Juan C., Norwich, CT, UNITED STATES Tucker, John L., Niantic, CT, UNITED STATES Zenoni, Maurizio, Milan, ITALY INVENTOR(S):

Fogliato, Giovanni, Bergamo, ITALY Donadelli, Alessandro, Lodi, ITALY

PATENT ASSIGNEE(S): Pfizer Inc. (U.S. corporation)

NUMBER	KIND	DATE	
US 2002099205 US 2001-6579	A1 A1	20020725 20011204	(10)

NUMBER DATE US 2000-251018P 20001204 (60) PRIORITY INFORMATION:

DOCUMENT TYPE: Utility APPLICATION FILE SEGMENT:

PFIZER INC, 150 EAST 42ND STREET, 5TH FLOOR -LEGAL REPRESENTATIVE:

STOP 49, NEW YORK, NY, 10017-5612

39 NUMBER OF CLAIMS: EXEMPLARY CLAIM: 1 1433 LINE COUNT:

> 308-4994 Searcher : Shears

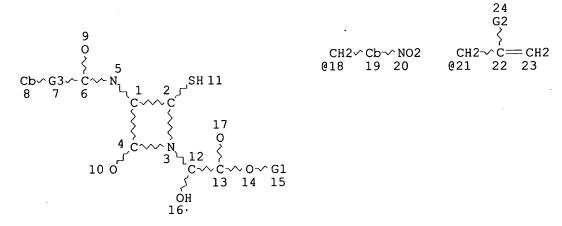
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates a process for preparing a compound of formula (I) ##STR1##

wherein R.sup.1 is para-nitrobenzyl or allyl; and X is halo, which is useful to prepare 3-cyclic-ether-substituted cephalosporins, from trimethylphosphinic compounds. This invention also relates to compounds useful in such process.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

(FILE 'MARPAT' ENTERED AT 15:46:35 ON 04 OCT 2002)
L7 STR



VAR G1=18/21
VAR G2=H/CH3
REP G3=(1-6) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 8
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC I NUMBER OF NODES IS 2

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:
MLEVEL IS CLASS ON RING NODES AND RING GROUPS
MLEVEL IS CLASS ON CHAIN NODES AND CHAIN GROUPS
ECLEVEL IS LIM ON ALL NODES
ALL RING(S) ARE ISOLATED

L14 SEA FILE=MARPAT SSS FUL L7 (MODIFIED ATTRIBUTES)

100.0% PROCESSED 26751 ITERATIONS (6 INCOMPLETE) 7 ANSWERS SEARCH TIME: 00.02.02

L14 ANSWER 1 OF 7 MARPAT COPYRIGHT 2002 ACS ACCESSION NUMBER: 137:33162 MARPAT

TITLE: Process for the preparation of p-nitrobenzyl or

allyl esters of 3-cyclic-ether substituted cephalosporins from trimethylphosphinic

compounds via an intramolecular Wittig reaction

Colberg, Juan Carlos; Tucker, John Lloyd;

Zenoni, Maurizio; Fogliato, Giovanni; Donadelli,

Alessandro

PATENT ASSIGNEE(S):

Pfizer Products Inc., USA PCT Int. Appl., 47 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

INVENTOR(S):

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.				KIND DATE					APPLICATION NO. DATE							
WO 2002046199			A1 20020613				WO 2001-IB2181 20011119									
	W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,
		LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,
		NO,	NZ,	OM,	PH,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,
		TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZW,	ΑM,	ΑZ,	BY,
		KG,	ΚZ,	MD,	RU,	ТJ,	\mathbf{MT}									
	RW:													ZW,		
		CH,	CY,	DE,	DK,	ES,	FΙ,	FR,	GB,	GR,	ΙE,	ΙT,	LU,	MC,	ΝL,	PT,
		SE,	TR,	BF,	ΒJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,
		SN,	TD,	TG												
AU 2002023929 A					5	20020618			AU 2002-23929 20011119							
US 2002099205				A	1 :	2002		US 2001-6579 20011204								
PRIORITY APPLN. INFO.: US 2000-251018P 20001204																
	WO 2001-IB2181 20011119															

OTHER SOURCE(S):

CASREACT 137:33162

GΙ

$$R^2$$
 NH S PMe_3 CO_2R^1 I

A process for the prepn. of I (R1 = p-nitrobenzyl, allyl; X = halo) AB

> 308-4994 Searcher : Shears

```
via an intramol. Wittig reaction of II (Rl = p-nitrobenzyl, allyl;
R2 = C1-6-alkyl, C6-10-aryl, C6-10-aryl-C1-6-alkyl, dithianyl) to
prep. 3-cyclic-ether substituted derivs. of cephalosporins is
described. Thus, III was treated with p-nitrobenzyl glyoxylate
monohydrate followed by redn. of the intermediate with NaBH4. The
resulting hydroxy compd. was treated with p-toluenesulfonic acid
followed by addn. of (S)-1-(tetrahydro-2-furanyl)ethanone, addn. of
thionyl chloride, and finally trimethylphosphine to give the desired
intermediate II (R1 = p-nitrobenzyl, R2 = PhCH2). Cyclization of II
via an intramol. Wittig reaction was accomplished by refluxing for
16 h in THF. Addn. of phosphorus pentachloride and .alpha.-picoline.
in dichloromethane gave the free amine of I (R1 = p-nitrobenzyl).
ICM C07D501-08
    C07D501-18; C07D501-20; C07D405-12; C07F009-568; C07D205-095;
ICS
     C07D513-04; C07D513-04; C07D277-00; C07D205-00
26-5 (Biomolecules and Their Synthetic Analogs)
cephalosporin lactam antibiotic cyclic ether substituted prepn;
Wittig reaction intramol cyclic ether cephalosporin prepn
Wittig reaction
   (intramol.; process for the prepn. of p-nitrobenzyl or allyl
   esters of 3-cyclic-ether substituted cephalosporins from
   trimethylphosphinic compds. via an intramol. Wittig reaction)
Lactams
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)
   (.beta.-; process for the prepn. of p-nitrobenzyl or allyl esters
   of 3-cyclic-ether substituted cephalosporins from
   trimethylphosphinic compds. via an intramol. Wittig reaction)
Antibiotics
   (.beta.-lactam; process for the prepn. of p-nitrobenzyl or allyl
   esters of 3-cyclic-ether substituted cephalosporins from
   trimethylphosphinic compds. via an intramol. Wittig reaction)
676-96-0
   (prepn. of)
               436100-74-2P
                              436100-75-3P
                                              436100-76-4P
436100-73-1P
               436100-78-6P
                              436800-38-3P
                                              436800-39-4P
436100-77-5P
436800-40-7P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
   (process for the prepn. of p-nitrobenzyl or allyl esters of
   3-cyclic-ether substituted cephalosporins from
   trimethylphosphinic compds. via an intramol. Wittig reaction)
               436800-42-9P
436100-68-4P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)
   (process for the prepn. of p-nitrobenzyl or allyl esters of
   3-cyclic-ether substituted cephalosporins from
   trimethylphosphinic compds. via an intramol. Wittig reaction)
                         67-56-1, Methanol, uses
                                                    67-64-1, Acetone,
64-17-5, Ethanol, uses
       68-12-2, DMF, uses
                            71-23-8, Propanol, uses
                                                       75-09-2,
uses
Methylene chloride, uses
RL: NUU (Other use, unclassified); USES (Uses)
   (process for the prepn. of p-nitrobenzyl or allyl esters of
   3-cyclic-ether substituted cephalosporins from
   trimethylphosphinic compds. via an intramol. Wittig reaction)
                           594-09-2, Trimethylphosphine 619-73-
03-69-0 64370-42-9, Allyl glyoxylate
79-37-8, Oxalyl chloride
                       34103-69-0
4-Nitrobenzylalcohol
                                           436800-46-3
                                                         436801-05-7
131328-27-3
             141194-61-8
                            192049-49-3
```

IC

CC

ST

ΙT

TΤ

ΙT

ΙT

TΤ

IT

IT

IT

```
436801-06-8
                   436801-07-9
                                  436801-08-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (process for the prepn. of p-nitrobenzyl or allyl esters of
        3-cyclic-ether substituted cephalosporins from
        trimethylphosphinic compds. via an intramol. Wittig reaction)
     81779-73-9P
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
     RACT (Reactant or reagent)
        (process for the prepn. of p-nitrobenzyl or allyl esters of
        3-cyclic-ether substituted cephalosporins from
        trimethylphosphinic compds. via an intramol. Wittig reaction)
     108-48-5, 2,6-Lutidine
                              109-02-4, N-Methylmorpholine 110-86-1,
IT
     Pyridine, reactions 288-32-4, Imidazole, reactions
                                                              507-16-4,
                      7719-09-7, Thionyl chloride 7719-12-2,
     Thionyl bromide
                               7789-60-8, Phosphorus tribromide
     Phosphorus trichloride
     RL: RGT (Reagent); RACT (Reactant or reagent)
        (process for the prepn. of p-nitrobenzyl or allyl esters of
        3-cyclic-ether substituted cephalosporins from
        trimethylphosphinic compds. via an intramol. Wittig reaction)
                                THERE ARE 6 CITED REFERENCES AVAILABLE FOR
REFERENCE COUNT:
                          6
                                THIS RECORD. ALL CITATIONS AVAILABLE IN
                                THE RE FORMAT
L14 ANSWER 2 OF 7 MARPAT COPYRIGHT 2002 ACS
(ALL HITS ARE ITERATION INCOMPLETES)
                          136:257270 MARPAT
ACCESSION NUMBER:
                          Methods of decreasing or preventing pain using
TITLE:
                          spicamycin derivatives
                          Borsook, David
INVENTOR(S):
                          The General Hospital Corporation, USA
PATENT ASSIGNEE(S):
                          PCT Int. Appl., 26 pp.
SOURCE:
                          CODEN: PIXXD2
DOCUMENT TYPE:
                          Patent
                          English
LANGUAGE:
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
                                            APPLICATION NO. DATE
                      KIND DATE
     PATENT NO.
                                            -----
                             -----
     WO 2002024146
                             20020328
                      A2
                                           WO 2001-US29371 20010920
         W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU,
             CZ, DE, DK, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID,
             IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MD, MG, MK, MN, MW, MX, NO, NZ, PH, PL, PT, RO, RU, SD,
             SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
                                             US 2000-234382P 20000920
PRIORITY APPLN. INFO.:
     Methods of providing pain relief by administering a water-sol.
AB
     deriv. of spicamycin. Methods of using pain mediation agents are
     also provided.
IC
     ICM A61K
CC
     1-11 (Pharmacology)
     pain spicamycin analgesia
ST
IT
     Body, anatomical
```

(back, pain; spicamycin derivs. for prevention and treatment of various pains)

IT Nerve, disease

(diabetic neuropathy; spicamycin derivs. for prevention and treatment of various pains)

Drug delivery systems IT

(implants; spicamycin derivs. for prevention and treatment of various pains)

IT Herpesviridae

(infection, neuropathy; spicamycin derivs. for prevention and treatment of various pains)

Drug delivery systems IT

(injections, i.v.; spicamycin derivs. for prevention and treatment of various pains)

TT Nerve, disease

(neuralgia; spicamycin derivs. for prevention and treatment of various pains)

ፐጥ Pancreas, disease

(neuropathy; spicamycin derivs. for prevention and treatment of various pains)

ΙT Pain

> (opioid-resistant; spicamycin derivs. for prevention and treatment of various pains)

TT Viscera

> (pain; spicamycin derivs. for prevention and treatment of various pains)

Drug delivery systems IT

(slow-release; spicamycin derivs. for prevention and treatment of various pains)

Analgesics TT

Human

(spicamycin derivs. for prevention and treatment of various pains)

ΙT 87099-85-2, Spicamycin

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(spicamycin derivs. for prevention and treatment of various pains)

L14 ANSWER 3 OF 7 MARPAT COPYRIGHT 2002 ACS

(ALL HITS ARE ITERATION INCOMPLETES)

ACCESSION NUMBER: 135:318706 MARPAT

TITLE: Preparation of halogenated 2-amino-5,6-heptenoic acid derivatives useful as nitric oxide synthase

inhibitors

Grapperhaus, Margaret L.; Sikorski, James A.; INVENTOR(S):

> Awasthi, Alok K.; Wang, Lijuan J.; Pitzele, Barnett S.; Hansen, Donald W., Jr.; Manning,

Pamela T.

Pharmacia Corporation, USA PATENT ASSIGNEE(S): PCT Int. Appl., 133 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

KIND DATE APPLICATION NO. DATE PATENT NO.

```
WO 2001078719
                                              WO 2001-US12258 20010413
                        A1
                              20011025
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH,
              CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH,
              GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ,
              PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU,
              TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE,
              TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD,
              TG
                              20020425
     US 2002049202
                        A1
                                              US 2001-835191
                                                                 20010413
                                              US 2000-197032P
PRIORITY APPLN. INFO.:
                                                                 20000413
     Halogenated 2-amino-5, 6-heptenoic acid derivs.
     R7N:CMeNHCH2CR1:CR2CH2CH2CH(NH2)C(0)J[R1, R2 = H, halo, alkyl,
     haloalkyl (at least one of R1 or R2 contains halogen); R7 = H, OH; J
     = OH, alkoxy, NR3R4, where R3 = H, alkyl, alkenyl, alkynyl and R4 =
     H, (un) substituted heterocyclyl] were prepd. for use as nitric oxide
     synthase (NOS) inhibitors. Thus, (2S,5E)-2-amino-6-fluoro-7-[(1-
     iminoethyl)amino]-5-heptenoic acid dihydrochloride was prepd. by a
     multistep procedure starting from L-glutamic acid and showed IC50
     values 0.36, 68, 3.6, and 0.1 .mu.M in hiNOS, hecNOS, hncNOS, and
     human cartilage assays, resp.
IC
     ICM A61K031-221
          A61K031-195; A61K031-41; C07C259-14; C07C229-30; C07D271-06;
     ICS
          C07D257-04
CC
     34-2 (Amino Acids, Peptides, and Proteins)
     Section cross-reference(s): 1, 7
     acetimidoylaminoheptenoic acid aminohalo prepn inhibitor nitric
ST
     oxide synthase; haloaminoheptenoic acid prepn inhibitor nitric oxide
     synthase; aminoheptenoic acid halo prepn inhibitor nitric oxide
     synthase; heptenoic acid haloamino prepn inhibitor nitric oxide
     synthase
IT
     Alcoholism
     Anti-inflammatory agents
     Antiarthritics
     Antirheumatic agents
     Antitumor agents
         (prepn. of halogenated aminoheptenoic acid derivs. useful as
        nitric oxide synthase inhibitors)
IT
     54-11-5, Nicotine
     RL: BAC (Biological activity or effector, except adverse); BSU
     (Biological study, unclassified); BIOL (Biological study)
         (prepn. of halogenated aminoheptenoic acid derivs. useful as
        nitric oxide synthase inhibitors)
                                      367967-70-2P
                                                      367967-71-3P
IT
     367967-68-8P
                     367967-69-9P
     367967-72-4P
                     367967-73-5P
                                      367967-74-6P
                                                      367967-75-7P
                                      367967-78-0P
                                                      367967-79-1P
                     367967-77-9P
     367967-76-8P
                                                      367967-83-7P
                                      367967-82-6P
                     367967-81-5P
     367967-80-4P
                                      367967-86-0P
                                                      367967-87-1P
                     367967-85-9P
     367967-84-8P
     367967-88-2P
     RL: BAC (Biological activity or effector, except adverse); BSU
     (Biological study, unclassified); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
         (prepn. of halogenated aminoheptenoic acid derivs. useful as
```

```
nitric oxide synthase inhibitors)
     125978-95-2, Nitric oxide synthase
IT
     RL: BPR (Biological process); BSU (Biological study, unclassified);
     BIOL (Biological study); PROC (Process)
        (prepn. of halogenated aminoheptenoic acid derivs. useful as
        nitric oxide synthase inhibitors)
     367968-17-0P
TΤ
     RL: BYP (Byproduct); PREP (Preparation)
        (prepn. of halogenated aminoheptenoic acid derivs. useful as
        nitric oxide synthase inhibitors)
                                           77-76-9, 2,2-Dimethoxy propane
IT
     56-86-0, L-Glutamic acid, reactions
     401-56-9, Ethyl chlorofluoroacetate
                                            696-63-9, p-
                           1000-84-6, Ethyl acetimidate
                                                           1074-82-4,
    Methoxybenzenethiol
     Potassium phthalimide 1499-55-4, L-Glutamic acid 5-methyl ester
                 4418-61-5, 5-Aminotetrazole
                                               52386-40-0
     2356-16-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of halogenated aminoheptenoic acid derivs. useful as
        nitric oxide synthase inhibitors)
                                 126587-35-7P
                   59279-60-6P
                                                 129599-92-4P
IT
     45214-91-3P
                    136904-77-3P
                                   144090-56-2P
                                                   192314-71-9P
     129600-92-6P
                    367967-89-3P
                                   367967-90-6P
                                                   367967-91-7P
     206128-03-2P
     367967-92-8P
                    367967-93-9P
                                   367967-94-0P
                                                   367967-95-1P
                    367967-97-3P
                                   367967-98-4P
                                                   367967-99-5P
     367967-96-2P
     367968-00-1P
                    367968-01-2P
                                   367968-02-3P
                                                   367968-03-4P
                    367968-05-6P
                                   367968-06-7P
                                                   367968-07-8P
     367968-04-5P
                                   367968-10-3P
                                                   367968-11-4P
     367968-08-9P
                    367968-09-0P
                    367968-13-6P
                                   367968-14-7P
     367968-12-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
     RACT (Reactant or reagent)
        (prepn. of halogenated aminoheptenoic acid derivs. useful as
        nitric oxide synthase inhibitors)
                               THERE ARE 8 CITED REFERENCES AVAILABLE FOR
REFERENCE COUNT:
                         8
                               THIS RECORD. ALL CITATIONS AVAILABLE IN
                               THE RE FORMAT
L14 ANSWER 4 OF 7 MARPAT COPYRIGHT 2002 ACS
(ALL HITS ARE ITERATION INCOMPLETES)
ACCESSION NUMBER:
                         134:366693 MARPAT
                         Preparation of bis(aminoalkyl- or
TITLE:
                         amidinophenoxy) arylene- and heteroatom-
                         interrupted alkanes and analogs as tryptase
                         inhibitors
                         Anderskewitz, Ralf; Braun, Christine; Hamm,
INVENTOR(S):
                         Rainer; Disse, Bernd; Jennewein, Hans Michael;
                         Speck, Georg
PATENT ASSIGNEE(S):
                         Boehringer Ingelheim Pharma K.-G., Germany
                         Ger. Offen., 36 pp.
SOURCE:
                         CODEN: GWXXBX
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         German
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                      KIND
                                            APPLICATION NO.
     PATENT NO.
                            DATE
                      ____
     DE 19955476
                                            DE 1999-19955476 19991118
                       Α1
                            20010523
     WO 2001036374
                       A2
                            20010525
                                           WO 2000-EP11216 20001114
     WO 2001036374
                       Α3
                            20020411
```

```
W: AE, AU, BG, BR, CA, CN, CZ, EE, HU, ID, IL, IN, JP, KR, LT,
             LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, US, UZ, VN, YU, ZA,
             AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC,
             NL, PT, SE, TR
PRIORITY APPLN. INFO.:
                                            DE 1999-19955476 19991118
     B1Z1X1Z2X2ZX3Z3X4Z4B2 [I; B1,B2 = C(:NR1)NHR1', CH2NH2, CH2CH2NH2,
     ureido; R1,R1' = OH, COR2, CO2R2; R2 = H, alkyl, aryl(alkyl); X1-X4
     = bond, CH2, CH2CH2, CH2O, CH2NH, etc.; Z = (heteroatom-
     interrupted) alkylene, G1(CH2)rG2 [X2 or X3 = (CH2)1-2], E1(CH2)rE2,
     etc.; E1,E2 = azacycloalkylene; G1,G1 = bond or cycloalkylene; Z1-Z4
     = (un) substituted (hetero) arylene; r = 0-6] were prepd.
     3-(C1H2C)C6H4CH2OC6H4(CH2CH2NHBoc)-4 was condensed with
     (CH2CMe2NH2)2 to give, after deprotection, the N,N'-bisbenzylated
     hexandiamine.4HCl. Data for biol. activity of I were given.
IC
     ICM C07C217-58
         C07C217-60; C07C213-02; C07D211-26; C07D295-12; C07C257-18;
     ICS
          C07C259-10; C07C271-62; C12N009-99; A61K031-155
     25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
CC
     Section cross-reference(s): 1
     azaarylenealkane bisaminophenoxy bisamidinophenoxy prepn tryptase
ST
     inhibitor; antiinflammatory azaarylenealkane bisaminophenoxy
     bisamidinophenoxy prepn; antiallergic azaarylenealkane
     bisaminophenoxy bisamidinophenoxy prepn
ΙT
     Allergy inhibitors
     Anti-inflammatory agents
        (prepn. of bis(aminoalkyl- or amidinophenoxy)arylene- and
        heteroatom-interrupted alkanes and analogs as tryptase
        inhibitors)
IT
     97501-93-4, Tryptase
     RL: BPR (Biological process); BSU (Biological study, unclassified);
     BIOL (Biological study); PROC (Process)
        (mediated disorders; treatment; prepn. of bis(aminoalkyl- or
        amidinophenoxy)arylene- and heteroatom-interrupted alkanes and
        analogs as tryptase inhibitors)
                                                   340284-45-9P
ΙT
     340284-41-5P
                    340284-43-7P
                                    340284-44-8P
                                                   340284-50-6P
     340284-46-0P
                    340284-48-2P
                                    340284-49-3P
                                    340284-53-9P
                                                   340284-54-0P
     340284-51-7P
                    340284-52-8P
     340284-55-1P
                    340284~56-2P
                                    340284-57-3P
                                                   340284-58-4P
                                                   340284-62-0P
     340284-59-5P
                    340284-60-8P
                                    340284-61-9P
                                                   340284-66-4P
     340284-63-1P
                    340284-64-2P
                                    340284-65-3P
                                                   340284-70-0P
     340284-67-5P
                    340284-68-6P
                                    340284-69-7P
                                                   340284-74-4P
     340284-71-1P
                    340284-72-2P
                                    340284-73-3P
     340284-75-5P
                    340284-76-6P
                                    340284-77-7P
                                                   340284-78-8P
     340284-79-9P
                    340284-80-2P
                                    340284-81-3P
                                                   340284-82-4P
     340284-83-5P
                    340284-84-6P
                                    340284-85-7P
                                                   340284-86-8P
                    340284-91-5P
                                    340284-92-6P
                                                   340284-93-7P
     340284-90-4P
                    340284-95-9P
                                    340284-96-0P
                                                   340284-97-1P
     340284-94-8P
                    340284-99-3P
                                    340285-00-9P
                                                   340285-01-0P
     340284-98-2P
     340285-02-1P
                    340285-03-2P
                                    340285-04-3P
                                                   340285-05-4P
                    340285-07-6P
                                    340285-09-8P
                                                   340285-10-1P
     340285-06-5P
                                                   340285-14-5P
                    340285-12-3P
                                    340285-13-4P
     340285-11-2P
                    340285-16-7P
     340285-15-6P
     RL: BAC (Biological activity or effector, except adverse); BSU
     (Biological study, unclassified); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (prepn. of bis(aminoalkyl- or amidinophenoxy)arylene- and
```

```
heteroatom-interrupted alkanes and analogs as tryptase
        inhibitors)
                                                  255915-70-9
IT
     23578-35-0, 2,5-Diamino-2,5-dimethylhexane
     340284-87-9
                   340284-88-0
                                 340284-89-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of bis(aminoalkyl- or amidinophenoxy)arylene- and
        heteroatom-interrupted alkanes and analogs as tryptase
        inhibitors)
L14 ANSWER 5 OF 7 MARPAT COPYRIGHT 2002 ACS
(ALL HITS ARE ITERATION INCOMPLETES)
                         131:5098 MARPAT
ACCESSION NUMBER:
TITLE:
                         Acylation of aromatic compounds
                         Baudry, Barbier Denise; Dormond, Alain; Richard,
INVENTOR(S):
                         Stephanie; Desmurs, Jean Roger
                         Rhodia Chimie, Fr.
PATENT ASSIGNEE(S):
                         Fr. Demande, 38 pp.
SOURCE:
                         CODEN: FRXXBL
DOCUMENT TYPE:
                         Patent
                         French
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                            DATE
     ------
                            19990326
                                                            19970919
                       A1
                                           FR 1997-11701
     FR 2768729
                         CASREACT 131:5098
OTHER SOURCE(S):
ΑB
     The title process takes place in the presence of, e.g., a rare earth
     halide. Thus, benzoylation of anisole gave 90.3% 4-(MeO)C6H4COPh in
     the presence of NdCl3.dioxane.
     ICM C07C049-76
IC
         C07C045-45; B01J027-125; B01J031-22
     ICS
    B01J031-22, B01J103-26
ICI
     25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
CC
     acylation arom rare earth catalyst; benzophenone prepn
ST
TΨ
     Ketones, preparation
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (arom.; acylation of arom. compds.)
IT
     Acylation catalysts
     Acylation catalysts
        (benzoylation catalysts; acylation of arom. compds.)
IT
     Benzoylation
     Benzoylation
        (catalysts; acylation of arom. compds.)
     611-94-9P, p-Methoxybenzophenone
                                        5672-94-6P, 1-Acetyl-2-
IT
                          5703-21-9P, 4-Acetylveratrole
     methoxynaphthalene
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (acylation of arom. compds.)
     91-16-7, Veratrole 93-04-9, 2-Methoxynaphthalene
                                                           98-88-4,
IT
                      100-66-3, Anisole, reactions
     Benzoyl chloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (acylation of arom. compds.)
                                         10361-92-9, Yttrium trichloride
     10024-93-8, Neodymium trichloride
     RL: CAT (Catalyst use); USES (Uses)
        (catalyst for acylation of arom. compds.)
```

L14 ANSWER 6 OF 7 MARPAT COPYRIGHT 2002 ACS (ALL HITS ARE ITERATION INCOMPLETES) ACCESSION NUMBER: 131:5097 MARPAT TITLE: Acylation of aromatic compounds Baudry, Barbier Denise; Dormond, Alain; Richard, INVENTOR(S): Stephanie; Bouazza, Aicha; Desmurs, Jean Roger PATENT ASSIGNEE(S): Rhodia Chimie, Fr. SOURCE: Fr. Demande, 28 pp. CODEN: FRXXBL DOCUMENT TYPE: Patent LANGUAGE: French FAMILY ACC. NUM. COUNT: PATENT INFORMATION: KIND DATE PATENT NO. APPLICATION NO. DATE ____ FR 2768728 A1 19990326 FR 1997-11700 19970919 TR 2/68728 B1 19991203
OTHER SOURCE(S): CASREACT 131 CASREACT 131:5097 The title process takes place in the presence of a U or uranyl halide. Thus, benzoylation of anisole gave 93% 4-(MeO)C6H4COPh after 1h reflux in the presence of a catalyst prepd. from U308 and HCl. IC ICM C07C049-76 ICS C07C049-786; C07C049-84; B01J027-08 ICI B01J027-08, B01J103-28 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds) CC acylation arom uranium catalyst; benzophenone prepn STKetones, preparation ΙT RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (arom.; acylation of arom. compds.) Acylation catalysts TΤ Acylation catalysts (benzoylation catalysts; acylation of arom. compds.) Benzoylation ΤТ Benzoylation (catalysts; acylation of arom. compds.) ΙT 134-84-9P 611-94-9P 954-16-5P 4044-60-4P 4885-14-7P 26086-67-9P 40777-50-2P 225780-54-1P 225780-55-2P 6317-73-3P RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (acylation of arom. compds.) ΙT 95-93-2, Durene 98-88-4, Benzoyl chloride 100-20-9, 1,4-Benzenedicarbonyl dichloride 100-66-3, Anisole, reactions 101-84-8, Diphenyl oxide 106-42-3, p-Xylene, reactions 108-67-8, Mesitylene, reactions 108-88-3, Toluene, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (acylation of arom. compds.) L14 ANSWER 7 OF 7 MARPAT COPYRIGHT 2002 ACS (ALL HITS ARE ITERATION INCOMPLETES) 130:196650 MARPAT ACCESSION NUMBER: TITLE: 2-Benzoylcyclohexane-1,3-diones as herbicides Engel, Stefan; Rheinheimer, Joachim; Baumann, INVENTOR(S): Ernst; Von Deyn, Wolfgang; Hill, Regina Luise; Mayer, Guido; Misslitz, Ulf; Wagner, Oliver; Witschel, Matthias; Otten, Martina; Walter,

Helmut; Westphalen, Karl-otto; et al.

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 81 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

GI

PATENT NO. KIND DATE								APPLICATION NO.						DATE		
WO	9910	327		A1 1999			0304		WO 1998-EP4634 1998080							
	W:	AL,	ΑU,	BG,	BR,	BY,	CA,	CN,	CZ,	GE,	HU,	ID,	IL,	JP,	KR,	ΚZ,
		LT,	LV,	MK,	MX,	NO,	ΝZ,	PL,	RO,	RU,	SG,	SI,	SK,	TR,	UA,	US,
							ΚZ,									
	RW:	ΑT,	BE,	CH,	CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙΤ,	LU,	MC,
		NL,	PT,	SE												
AU	9890	684		A.	1	1999	0316		Α	J 19	98-90	0684		19980	0805	
EP	1001	938		A.	1	2000	0524		EI	P 19	98-94	4261	l	19980	0805	
	R:	CH,	DE,	FR,	GB,	LI							•			
JP	2001	5141	71	T	2	2001	0911		JI	P 20	00-50	0765	5	19980		
ZA	9807	057		Α		2000	0207		\mathbf{z}_{I}	A 19	98-70	057		19980	0806	
US	6432	381		B:	1	2002	0813		US	3 20	00-48	3523	l	20000	0207	
PRIORITY	APP	LN.	INFO	. :					DI	E 19	97-19	9734:	164	19970	0807	
									W	19	98-E	P4634	4	19980	0805	

$$Q-CO$$
 XR
 Me
 Me
 CO
 SO_2Me
 II

- AB The 2-benzoylcyclohexane-1,3-diones I [Q = (un)substituted 1,3-dioxo-2-cyclohexyl; X = nalkylene, oxaalkylene, thiaalkylene; R = heterocyclic; R1, R2 = H, NO2, halogen, CN, SCN, (un)substituted alkyl, OH, SH, SO3H, SO2NH2, NHSO2H, acylamino] were prepd. for use as herbicides (no data). Thus, Me 2-chloro-3-methyl-4-methylsulfonylbenzoate was treated with 1-methyl-5-pyrazolol, hydrolyzed to the acid and treated with dimedone to give the benzoylpyrazole II.
- IC ICM C07D231-12 ICS C07D231-14; A01N043-56
- CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 5
- ST benzoylcyclohexanedione prepn herbicide; pyrazolylbenzoylcyclohexanedione prepn herbicide; pyridylbenzoylcyclohexanedione prepn herbicide
- IT Herbicides
- (prepn. of benzoylcyclohexanediones as herbicides)
 IT 220798-99-2P 220799-06-4P 220799-10-0P 220799-15-5P

220799-18-8P 220799-24-6P 220799-29-1P 220799-33-7P RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of benzoylcyclohexanediones as herbicides)

IT 126-81-8, Dimedone 33641-15-5, 5-Hydroxy-1-methylpyrazole 120100-04-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of benzoylcyclohexanediones as herbicides)

IT 120100-44-9P 220798-89-0P 220798-93-6P

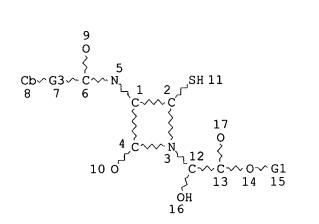
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)

(prepn. of benzoylcyclohexanediones as herbicides)

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

FILE MARPATPREV' ENTERED AT 15:49:55 ON 04 OCT 2002 L7 STR



24 G2 \$ CH2\sqrt{Cb\sqrt{NO2}} CH2\sqrt{C}\def CH2 @18 19 20 @21 22 23

VAR G1=18/21
VAR G2=H/CH3
REP G3=(1-6) C
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 8
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:
MLEVEL IS CLASS ON RING NODES AND RING GROUPS
MLEVEL IS CLASS ON CHAIN NODES AND CHAIN GROUPS
ECLEVEL IS LIM ON ALL NODES
ALL RING(S) ARE ISOLATED

0 SEA FILE=MARPATPREV SSS FUL L7 (MODIFIED ATTRIBUTES)

100.0% PROCESSED 127 ITERATIONS

O ANSWERS

SEARCH TIME: 00.00.06

=> fil hom

FILE 'HOME' ENTERED AT 15:50:21 ON 04 OCT 2002